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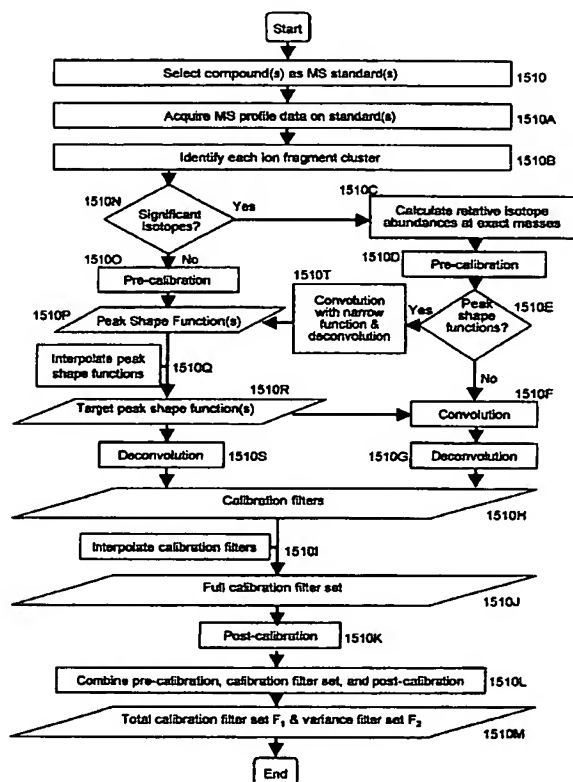
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(54) Title: METHODS FOR CALIBRATING MASS SPECTROMETRY (MS) AND OTHER INSTRUMENT SYSTEMS AND
FOR PROCESSING MS AND OTHER DATA



(57) Abstract: A method for obtaining at least one calibration filter for a Mass Spectrometry (MS) instrument system. Measured isotope peak cluster data in a mass spectral range is obtained for a given calibration standard. Relative isotope abundances and actual mass locations of isotopes corresponding thereto are calculated for the given calibration standard. Mass spectral target peak shape functions centered within respective mass spectral ranges are specified. Convolution operations are performed between the calculated relative isotope abundances and the mass spectral target peak shape functions to form calculated isotope peak cluster data. A deconvolution operation is performed between the measured isotope peak cluster data and the calculated isotope peak cluster data after the convolution operations to obtain the at least one calibration filter. Provisions are made for normalizing peak widths, combining internal and external calibration, and using selected measured peaks as standards. Aspects of the methods are applied to other analytical instruments.



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